Two-point distance distribution of knotted ring polymers at the theta temperature and a topological correction

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線状高分子鎖の末端間距離分布に相当する環状高分子鎖の2点間分布が、結び目の制限からどのような影響を受けるかを議論する。また、この分布に対する近似式もシミュレーション結果から考察する。

1 Introduction

In 1979 des Cloizeaux proposed an interesting conjecture that a topological constraint should lead to effective repulsion among segments of ring polymers so that the mean size of very long ring polymers should swell under the topological constraint [1]. The conjecture is supported by some computer simulations [2, 3, 4, 5, 6, 7]. At the Θ temperature ring polymers balance between attractive and repulsive forces among segments of them. Although they have in principle no excluded volume, topological repulsion remains under topological constraints. Thus, the mean size of ring polymers of no thickness swells under topological constraints as if they have the excluded volume.

Is a topologically repulsive effect the same as the excluded volume effect ? The answer is "No". The distribution of distance between opposite nodes of random polygons under topological constraints is nearly the Gaussian distribution rather than the end-to-end distance distribution of self-avoiding walks [8]. This suggests that random polygons under topological constraints do not behave almost like a self-avoiding walk. Here, a random polygon means a random walk with closing ends and this is an useful mathematical model of a ring polymer in solution at the Θ temperature.

In this work we consider not only a distance distribution between opposite nodes but also that of given a pair of nodes of random polygons. We find that these distributions are given by deformed Gaussian ones with additional topological correction terms.

2 Two-point distance distribution and Topological corrections

We consider a distance of a random polygon corresponding to an end-to-end distance of a random walk. Choose two nodes among N nodes of a random polygon with length N. Let m be the length along the short curve between the pair of nodes of the random polygon. The other length

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along the curve is $N - m$. The two curves have the same end-to-end distance. We call it the two-point distance of the random polygon.

Let us introduce the λ parameter which is a normalized length of pair nodes: $\lambda = m/N$ $(0 < \lambda \leq 1/2)$. Two-point distances belong to λN length of N-noded random polygons form a distribution corresponding to an end-to-end distance distribution of random walks. We observe two-point distance distributions of random polygons with length N changing λ from 1/20 to 1/2.

The distributions are given by almost the Gaussian distribution for all knot types when λ is very small. On the other hand the distribution for each knot K slightly differ from the Gaussian distribution when λ is nearly one-half. A two-point distance distribution of random polygon with knot type K is given by

$$f_K(r; \lambda, N) = A_K r^{2+\theta_K} \exp\left[-\frac{3r^{\delta_K}}{2{\sigma_K}^2(\lambda)N}\right], \tag{1}$$

where θ_K, δ_K and ${\sigma_K}^2(\lambda)$ are topological corrections. Here we note that if θ_K, δ_K and ${\sigma_K}^2(\lambda)$ hold 0, 2 and $\sqrt{\lambda(1-\lambda)}$ respectively, $f_K(r; \lambda, N)$ is exactly the Gaussian distribution. Our simulation imply that the exponent δ_K is given by two for any knot and any λ. Topological effects increase the exponent θ_K and the dispersion ${\sigma_K}^2(\lambda)$ when λ increasing; $0 < \lambda \leq 1/2$.

Acknowledgment

The author would like to thank Professor Tetsuo Deguchi for valuable discussions and comments.

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